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SEMIANNUAL TECHNICAL STATUS REPORT,
FEBRUARY 1972 THROUGH JULY 1972

A. V. Phelps, et al

Joint Institute for Laboratory Astrophysics

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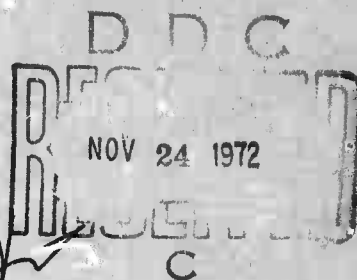
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I. MODELING OF IONIZED GAS SYSTEMS;

Program Leader - Dr. A. V. Phelps

Our studies of the modeling of ionized gas systems include a) the theoretical prediction of the conditions for the growth of a constriction in a weakly ionized gas, such as found in a molecular gas laser; b) the development of theories of radiation transport and hydrodynamics applicable to a wider variety of real situations, such as expanding and turbulent plasmas in geometries other than the usual planar geometry; c) the testing of radiative transport theories under controlled laboratory conditions; and d) the experimental determination of the laws of radiative scattering and absorption appropriate to radiative transport problems. The overall objective of this program is to supply experimentally tested understanding and computational techniques required for the analysis and prediction of the role of a) the generation and transport of radiation in plasmas and b) the transport and reactions of charged particles in weak to fully ionized gases. Because of its concern with a number of simultaneous atomic processes and with relatively large numbers of interacting atoms or molecules, this program also provides an important link between the experimental and theoretical determinations of cross sections and rate coefficients which make up much of the remainder of the program and the technology of ionized and excited gases which this work is designed to support.

Stability of Discharges in Weakly Ionized Gases (Dr. E. F. Jaeger, Dr. L. Oster and Dr. A. V. Phelps)

The objective of this theoretical project is the quantitative investigation of factors which control the growth of instabilities in weakly ionized gas discharges, such as used in high power molecular lasers. The present phase of this project is concerned with instabilities which result from a decrease in gas density and the accompanying increase in the ratio of the electric field to the gas density E/N and in the rate of ionization.

Since the arrival of Dr. Jaeger in June, we have been investigating the predictions and validity of previously published solutions for the steady state spatial distributions of electron density and gas temperature and for the stability of these solutions against fluctuations in discharge conditions. We find agreement with previous results only if one takes into account the high degree of sensitivity of the results to changes in the material properties, such as the ambipolar diffusion and ionization coefficients. An example of this sensitivity is shown in Fig. 1 where the spatial distribution of the electron density for a helium discharge is plotted as a function of radius for various assumed variations of the ambipolar diffusion coefficient with E/N or equivalent variable ET/p . The value of $n = 1/3$ is most nearly correct for helium in the usual range of E/N , although n varies significantly among gases.

In addition, we have obtained solutions for the time dependence of the electron density, gas temperature, discharge current and electric field for a range of applied voltages, source impedances, etc. Some of these results are shown in Fig. 2 for a discharge in helium with values appropriate to a low pressure, moderate current discharge. Unfortunately, an

examination of the neutral atom density profiles for this case shows that the gas is expanding with a velocity which far exceeds the velocity of sound appropriate to the peak temperature. This calculation confirms our original justification of this project, i.e., that the constant pressure approximation normally used in modeling glow discharges should not be used at times, pressures and dimensions of interest in many laser problems. We are currently formulating the hydrodynamic and charged particle equations appropriate to these discharges.

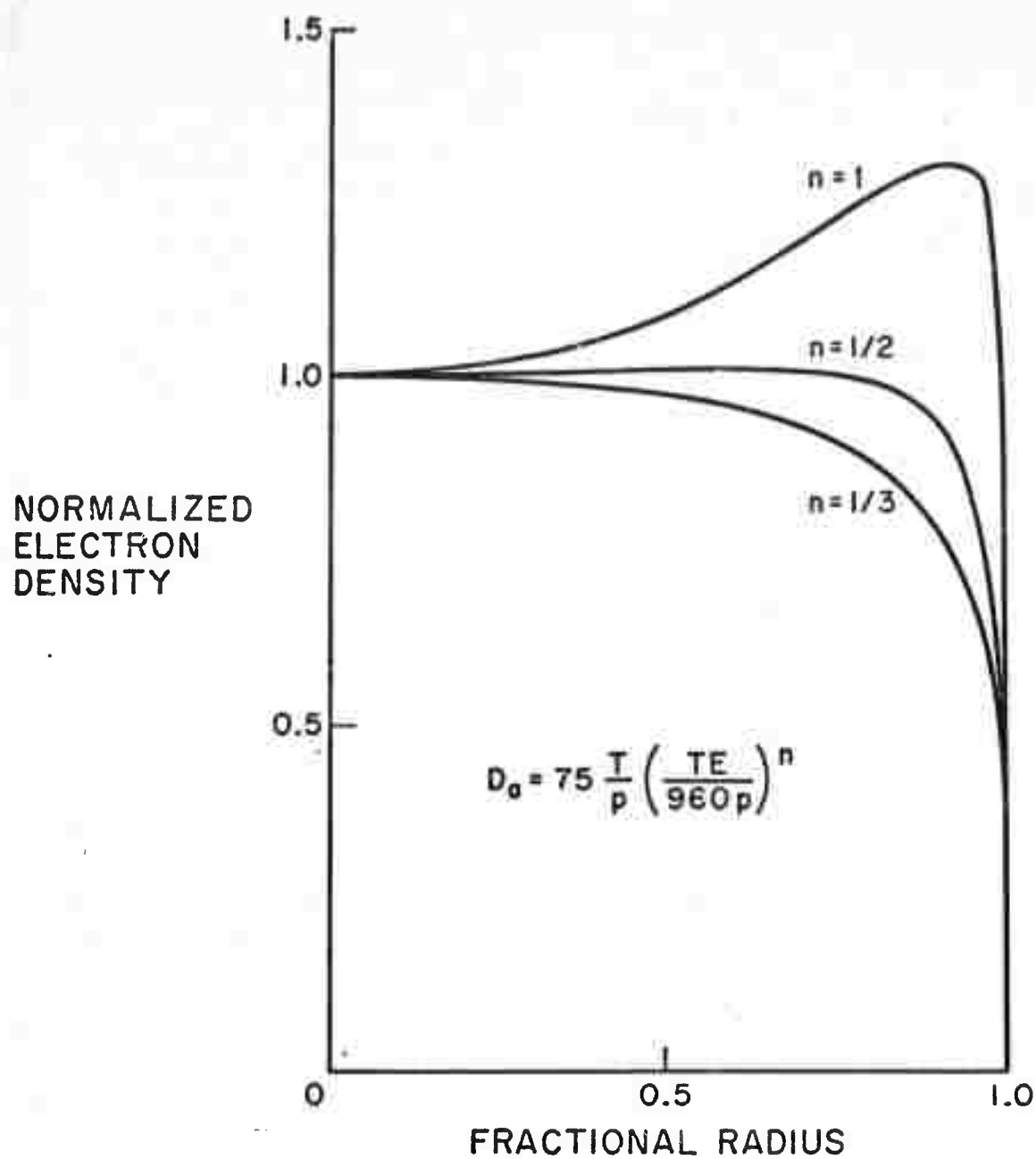


Fig. 1. Effects of variations in ambipolar diffusion coefficient on steady state electron density.

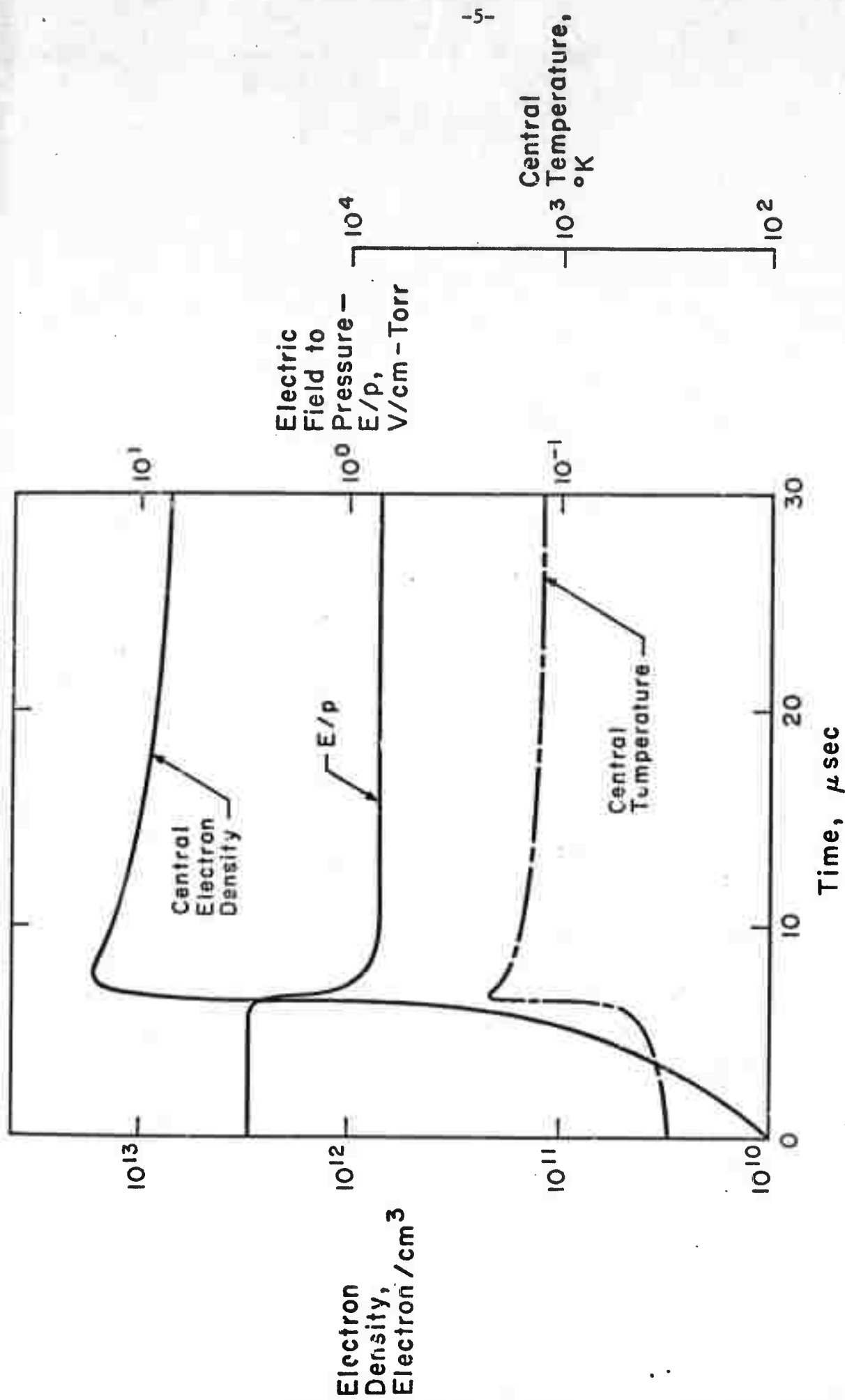


Fig. 2. Time variation of electron density, E/p and temperature for helium discharge.
 $pR = 10 \text{ Torr-cm}$, $I_{ss} = 30 \text{ A-Torr}$.

Scattering and Transport of Resonance Radiation (Dr. A. V. Phelps and Dr. J. V. Jenkins)

During the period of this report we have completed a set of measurements of the line profiles of the first resonance doublet of potassium at moderately high densities. We have been especially concerned with the accuracy to which the density of potassium vapor can be calculated from the equilibrium vapor pressure data. In order to test the equilibrium data, measurements have been made of the intensity of radiation reflected from the interface between the potassium vapor and the glass window. The magnitude of the reflection coefficient in the wings of the profile is a measure of the product of the ground state atom density and the oscillator strength for the resonance line. Using other measurements of the oscillator strength one can determine the ground state density. Alternately, one can use the equilibrium vapor pressure data and oscillator strength data to predict the reflection coefficient. Figure 3 shows such a comparison for the 7644 Å line of potassium. Because of some discoloration of the windows as the result of reactions between the potassium and the glass (Corning 1720), there is some uncertainty in the dielectric coefficient of the glass. We are therefore repeating the measurements with an optical arrangement which allows much more rapid collection and intercomparison of data.

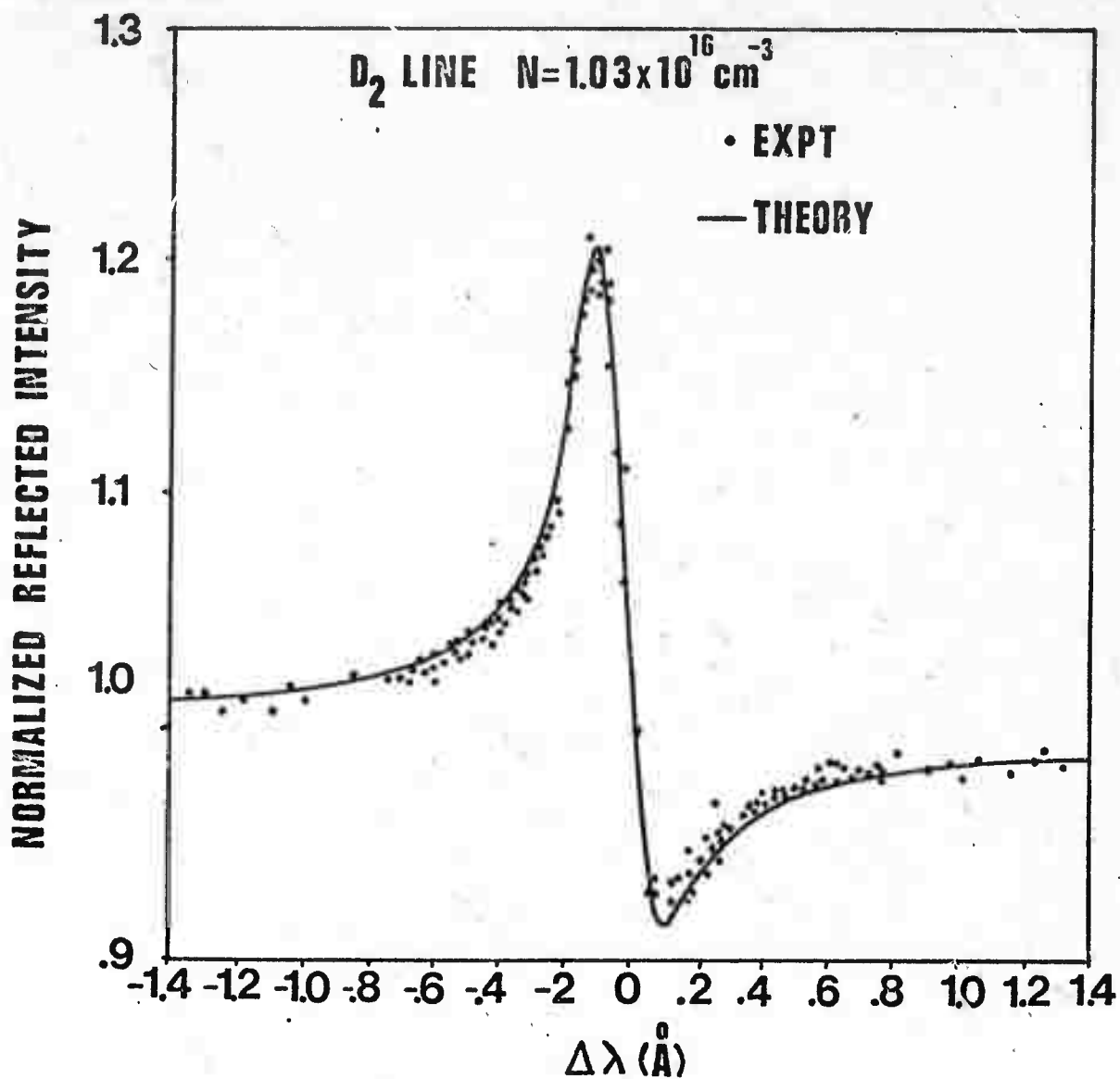


Fig. 3. Experimental and theoretical specular reflection profiles for 6944 Å line of potassium.

Radiative Hydrodynamics (Dr. D. G. Hummer, Dr. J. Cassinelli, Dr. J. Castor and Mr. P. Kunasz)

Line formation in spherical geometry. The important problem of spectral line formation in a spherical emitting cloud is complicated by the existence of three characteristic scale lengths, which may be taken as line center total optical thickness, the thermalization length and the radius of curvature. In more conventional plane parallel configuration only the first two are encountered, and the situations occurring when one or the other is the larger are well understood. However, for the spherical case very little is understood about the regime defined by a specific ordering of these characteristic lengths.

As an aid in understanding the line formation process in spherical configurations as well as to provide the capability for accurately computing the line radiation field in these geometries, we have generalized the non-linear iteration procedure reported earlier (the so-called variable Eddington factor method) for monochromatic transfer^{1,2} to allow for non-conservative transfer in a gas in which the opacity varies with frequency. The coupling of radiation of different frequencies because of non-coherent scattering is taken into account. Coupled differential equations for the monochromatic mean intensity, containing the Eddington factors have been derived and a suitable difference scheme has been devised. A code embodying this analysis has been written and is now being tested. Some trouble has been encountered in situations in which the optical depth is very small and the ratio of outer to inner radii is very large. The solution of the difficulty is now being pursued.

In conjunction with the studies on line formation, the subroutine FORMAL, which computes the formal solution of any spherical transfer pro-

blem (given the opacity and source function as functions of radius, this subroutine evaluates the radiation field and its first three moments) has been completely rewritten for increased accuracy and speed, and can now operate with much less storage, because of improved logic and a more accurate difference scheme. An account of this subroutine is being prepared for publication in Computer Physics Communications.

Radiative transfer in a doublet in the presence of excited atom diffusion. As a further extension of our study of radiative transfer phenomena in laboratory situations, we have generalized our previous analysis of radiative transfer in a spectral line in situations where the diffusion of the excited atoms is important to the case of a spectral doublet. We had earlier also solved the doublet transfer problem without excited-state diffusion. Because of the very great complexity of the present problem, the analysis will not be coded until a clear indication of the need for these results is forthcoming.

The results obtained from earlier work on these problems is now being prepared for publication and the possibility of publishing a set of computer codes for laboratory radiative transfer is being investigated.

Radiation hydrodynamics in spherical geometries. The transfer of radiation in a spherically symmetric moving medium has been considered including terms of order v/c , where v is of the order of the flow velocity, using a formulation in which the radiation quantities are those in the fluid frame. The lowest frequency-integrated movement equation is equivalent to the first law of thermodynamics for the radiation and its use insures that the internal energy and radiation pressure is correctly accounted for in the conservation of energy for the whole system. The fluid equations including the effects of matter-radiation coupling and total energy con-

servation have been derived in a form which shows that the difference between the fluid frame and stationary frame values of the radiative flux can be regarded as the convective flux of radiation enthalpy. This work corrects some errors in earlier treatments of this problem. Some novel approximations that could be applied to various forms of the transfer equation to make them computationally tractable have been discussed and are currently being investigated, including further generalizations of the variable Eddington-factor method.

References

1. D. G. Hummer and G. B. Rybicki, Monthly Notices Roy. Astron. Soc. 152, 1 (1971).
2. J. P. Cassinelli and D. G. Hummer, Monthly Notices Roy. Astron. Soc. 153, 9 (1971).

Plasma Statistics (Dr. W. E. Brittin and Dr. W. R. Chappell)

Dr. Chappell is presently developing a more general kinetic theory of Stark broadening of spectral lines in order to refine and extend the results obtained previously in collaboration with Dr. Cooper of JILA and Dr. Smith of NBS.¹ This work involves developing a kinetic equation for the dipole density autocorrelation function in a manner similar to that used for neutral gas broadening.² This work should give a better understanding of the effects of charged particle correlations. A paper with R. H. Williams was recently published in Physics of Fluids.³

References

1. W. R. Chappell, J. Cooper, and E. W. Smith, "Non-thermal Effects in Stark Broadening," J. Quant. Spectrosc. Radiative Transfer 10, 1195 (1970).
2. W. R. Chappell, J. Cooper, E. W. Smith, and T. Dillon, "A Kinetic Theory of Spectral Line Shapes," J. Stat. Phys. 3, 401 (1971).
3. W. R. Chappell and R. H. Williams, "Microscopic Theory of Conductivity of a Weakly Ionized Plasma," Phys. Fluids 15, 1059 (1972).

II. TRANSPORT COEFFICIENTS AND REACTION RATES, to p. 19

Program Leader - Dr. S. J. Smith

The prediction of the performance characteristics of ionized gas devices, such as the efficiency, power output and stability of high power lasers, requires that one be able to calculate accurate values of electron transport and reaction rate coefficients for electrons and ions. In order to meet some of these requirements we are engaged in: a) a determination of sets of electron collision cross sections consistent with measured electron transport and ionization coefficients and with recent electron beam measurements of excitation cross sections for the upper excited states of gases found in molecular lasers; b) measurement of cross sections for molecular dissociation; c) evaluation and compilation of low energy electron, photon, and ion collision cross section data; and d) determination of negative ion characteristics, such as single and multiple photodetachment cross sections, negative ion stability and low electron energy scattering parameters.

Electron Transport and Ionization Coefficients (Dr. G. E. Chamberlain,
Dr. L. J. Kieffer and Dr. A. V. Phelps)

For the past six months our efforts have been concentrated on the development of criteria to be used in the selection of a critical set of experimental electron transport coefficients. Emphasis is being placed on data for N_2 and on high values of E/N for which electronic excitation and ionization are important. (E = electric field, N = gas number density.) The Information Center bibliography and compilation of swarm data being prepared by J. Dutton has helped extensively. Criteria for selection of drift velocity data W are currently being summarized. The drift velocity work will be followed by the analysis and summary of criteria for selection of data on D/μ (ratio of diffusion to mobility coefficients), and α_i (ionization coefficient).

Our review of the literature shows that one now has a rather high degree of understanding of errors in electron drift velocity measurements caused by the diffusion of electrons along density gradients resulting from absorbing boundaries, ionization growth and electron injection and observation techniques. Unfortunately, only a few experimentalists have applied these corrections or have given sufficient information regarding experimental conditions so that we can apply the corrections. It appears that the situation is somewhat less satisfactory with regard to the effects of space charge, although our investigation is continuing. It should be noted that the careful formulation of all of the sources of error in transport coefficient determinations is not available at present so that this effort will aid others in making more reliable measurements as well as aid us in selecting data for use in our cross section analysis.

A second activity during this reporting period has been intercom-

parison of excitation and transport coefficients calculated at various laboratories for electrons in gas mixtures typical of electron beam sustained lasers, i.e., $\text{He:N}_2:\text{CO}_2 = 3:2:1$. The objectives of such a comparison are to determine whether the various methods for solving the relevant Boltzmann equation are equally accurate, to insure that the various groups are using the best available sets of electron scattering and excitation cross sections and to establish communication with the various groups so that improvements in cross sections or computational techniques can be distributed rapidly. Intercomparisons of the results of our calculations with those of three other laboratories showed one set of results to be in very good agreement with ours, one with up to 20% too large a rate of vibrational excitation and one with as much as 10% too low a rate of vibrational excitation. Sources of the low rate of excitation are being investigated through further calculations by the laboratory involved.

JILA Information Analysis Center (Dr. L. J. Kieffer)

The Information Center prepared a report on the ARPA-supported Workshop "Dissociative Excitation of Simple Molecules" which was held 16-17 March, 1972. The report, issued as JILA Information Center Report No. 12, is available from the Defense Documentation Center, Cameron Station, Alexandria, Virginia 22314. The order number for this report is AD745417.

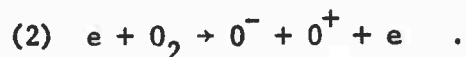
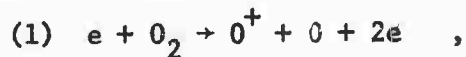
In addition to abstracts of most of the invited papers, the report contains an extensive compilation of cross section data for dissociative excitation of atmospheric molecules by electron impact and a discussion of the molecular branching ratio method for calibration of optical systems in the vacuum ultraviolet.

Work continues on the publications mentioned in the last semi-annual report. The publications will be reported when available.

Assistance continues to be given to Dr. A. V. Phelps in his attempt to obtain a "best set" of N_2 cross sections for use in laser modeling and modeling of other devices involving low pressure ionized gases.

Molecular Dissociation Processes (Dr. L. J. Kieffer)

During the month of July, Professor R. J. Van Brunt, University of Virginia (Visiting Scientist at JILA), took extensive data on two dissociative processes:



The angular distributions of the ion fragments as a function of both the ion energy and the electron energy for both these processes were observed. Also observed was the energy distribution of the O^- ions for process (2) (pair formation) as a function of the electron impact energy. The results of these experiments and data taken previously will be prepared for publication within the next six months.

Negative Ion Kinetics (Dr. W. C. Lineberger, Dr. J. Hall, Dr. H. Hotop, Mr. R. A. Bennett, Mr. T. A. Patterson and Mr. R. A. Beyer)

We have continued the studies of metallic negative ions produced in our sputtering ion source. Photodetachment of Au^- and Pt^- has been studied using a tunable dye laser with a $1\text{-}2\text{ \AA}$ bandwidth. The threshold behavior of the photodetachment cross section is that for outgoing p-wave electrons, and agrees with the Wigner threshold law, $\sigma \propto k^3$ over at least 50 meV above threshold. These data show that there are at least 2 states of Pt^- , and thus that the $d^9 s^2(^2D)$ configuration is stable. Hartree-Fock estimates by Weber at Northwestern indicate that the $d^{10} s(^2S)$ configuration of Pt^- is probably unstable. The results are that $\text{EA}(\text{Pt}) = 2.128 \pm .002\text{ eV}$ and that $\text{EA}(\text{Au}) = 2.3086 \pm .0007\text{ eV}$.

In a separate experiment we have attached our sputtering source to the laser-photoelectron spectroscopy apparatus of Dr. J. Hall, in which one measures the energy spectrum of electrons detached from a negative ion beam by an argon ion laser. The electron affinities of Ag^- and Cu^- were measured relative to O^- and OH^- respectively; the Cu^- detached electron energy spectrum is shown in Fig. 4. Our results are that $\text{EA}(\text{Ag}) = 1.303 \pm .008\text{ eV}$ and $\text{EA}(\text{Cu}) = 1.226 \pm .008\text{ eV}$. All of these electron affinities are $\sim 0.5\text{ eV}$ less than surface ionization measurements, and the $\text{EA}(\text{Cu})$ is $\sim 0.6\text{ eV}$ less than estimates based on accurate Hartree-Fock calculations with an empirical electron correlation correction added. These data, which represent the first accurate determinations of electron affinities of transition and noble metals, make it clear that many present estimates of electron affinities are incorrect. We hope to measure a number of additional electron affinities of metals in the near future.

We have also used the tunable dye laser to investigate photodetachment of OH^- and OD^- in the range $7000\text{\AA} - 6400\text{\AA}$. A detailed analysis of the observed cross sections is being made on the basis of the known term values for OH and OD ($X^2\Pi_1$) and the experimental result of Hall, Celotta and Bennett that $\gamma_e(\text{OH}^-, \text{OD}^-) = \gamma_e(\text{OH}, \text{OD})$ to within $\pm 0.001\text{\AA}$. The electron affinities are found to be $\text{EA}(\text{OH}) = 1.826 \pm .002 \text{ eV}$, and $\text{EA}(\text{OD}) = 1.823 \pm .002 \text{ eV}$. These values are in agreement with Branscomb's result of $1.83 \pm .04 \text{ eV}$ as extracted from a low resolution experiment.

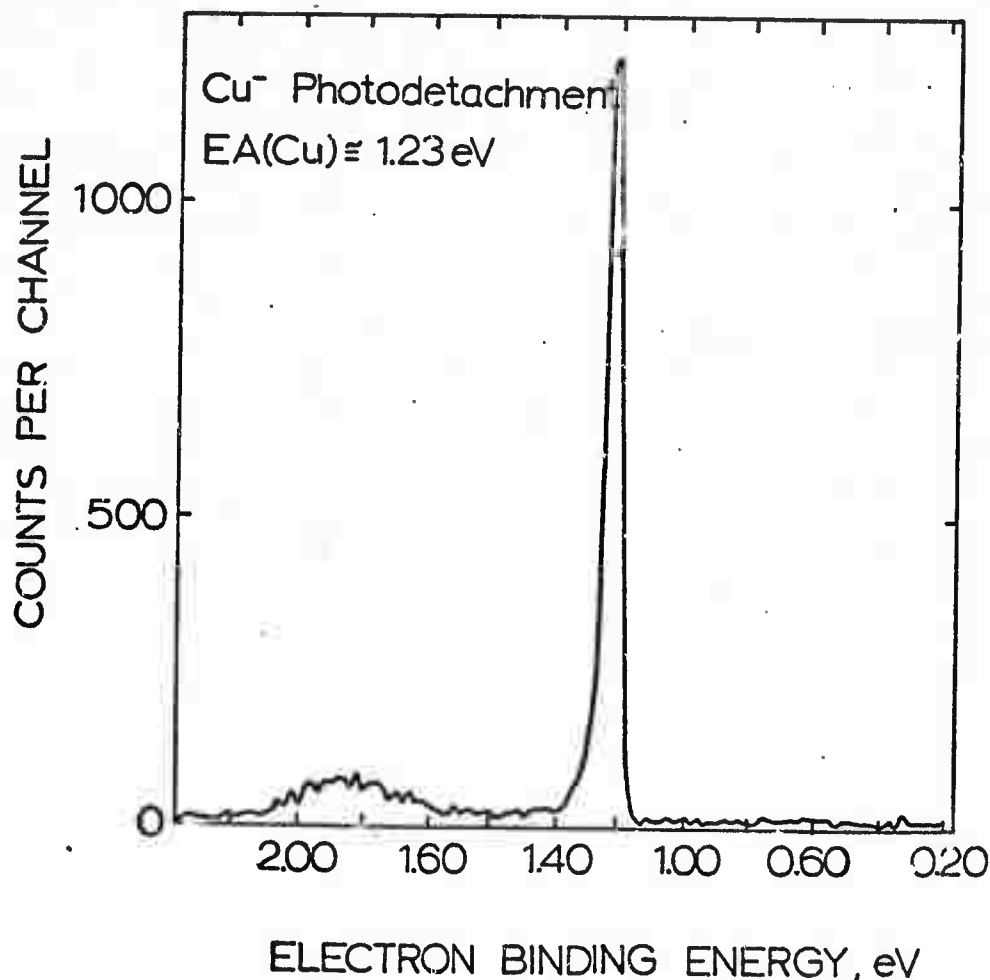


Fig. 4. Electron energy spectrum for electrons detached from Cu^- ions by 4880 \AA photons.

III. ENERGY LOSS AND RADIATION PRODUCTION BY ELECTRON COLLISIONS

Program Leader - Dr. E. C. Beaty

Interaction of Electrons with Ions (Dr. G. H. Dunn, Dr. F. L. Walls, Dr. D. Crandall and Mr. P. O. Taylor)

The interactions of electrons with ions can be very important in partially ionized gases because of the very large cross sections for scattering, excitation and dissociative recombination. We are engaged in measurements of excitation cross sections and recombination coefficients for ions of atmospheric interest and of importance for testing theory. The energy dependence of electron-molecular ion recombination coefficients has taken on added importance with the development of electron beam excited and sustained lasers.

The cross sections for electron-impact excitation of N_2^+ , Ca^+ , and Ba^+ are measured using crossed beams of variable energy electrons and the respective ions. The resultant resonance radiation is observed along the third perpendicular direction. Preliminary results were reported earlier. During this report period absolute radiometry was completed for the measurements cited above. Final cross section measurements were made on Ca^+ from 2 eV to 700 eV, and corrections to the data were carefully analyzed and applied. Figure 5 shows a plot of cross section versus electron energy for both the H ($4^2P_{1/2} \rightarrow 4^2S_{1/2}$) and K ($4^2P_{3/2} \rightarrow 4^2S_{1/2}$) emissions at 3968 and 3934 Å respectively. The measurements are absolute, and the flags represent 98% confidence limits (about 3 standard deviations). Points plotted with a B represent the three-state close coupling calculation of Burke and Moores.¹ Points plotted with S represent a Coulomb distorted wave calculation of Burgess and Sheory.² The measure-

ments indicate that further theory and/or computation is needed before such calculations can be trusted to within 30% in the threshold region where such cross sections are of value in understanding various plasmas.

Figure 6 shows a plot of the measured polarization for the K line as a function of electron energy. The points plotted with an S are due to a calculation by Saraph using Burke and Moores close-coupling matrix elements. Here the flags represent one standard deviation of statistical fluctuations combined with systematic uncertainties. Again the measurements indicate a need for further theoretical development. Work is continuing on the Ba^+ and N_2^+ measurements.

The experiment for measuring the energy dependence of electron molecular ion recombination coefficients employs trapping of ions in a dc electric and magnetic field configuration to investigate collisions of these ions with other particles. In particular dissociative recombination of these ions with monoenergetic electrons will be investigated over an electron energy range from 0 to several eV. This report period was spent in apparatus improvements looking forward to serious data taking. A new trap was fabricated from molybdenum, and its closer shape tolerance and low, uniform surface potentials should result in a device with narrower line widths. An interface was designed for running the experiment with a small computer, and programs were written to do so. Extra pumping was added to the system both in the form of liquid air trapping and Ti sublimation pumping. This resulted in a base pressure of 2×10^{-11} torr, increased ion residence times, and decreased ion-molecule reactions to an apparently acceptable level. Apparatus was assembled for testing the Channeltron bundle detector designed to measure the spatial distribution of ions in the trap.

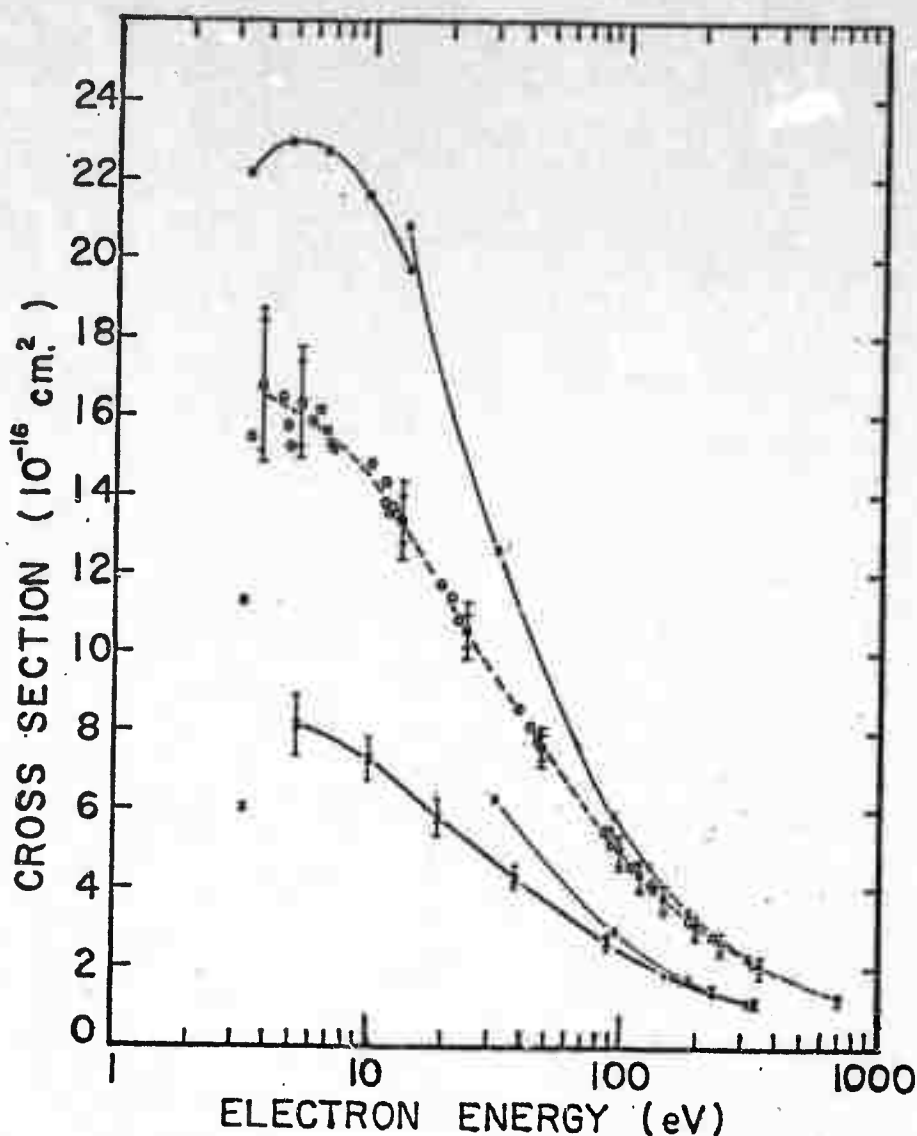


Fig. 5. Absolute cross sections for exciting the K and H emissions.

Present Experiment	0	K line	$\sigma(V_C - \phi - \Delta V)$
	■	K line	$\sigma(V_C - \phi)$
	X	H line	$\sigma(V_C - \phi - \Delta V)$
Theory	B	Close coupling calculation of Burke and Moores (Ref. 1).	
	S	Coulomb distorted wave calculation of Burgess and Shee (Ref. 2).	

The outer error bar on the experimental results represents the uncertainty in the absolute cross sections, including systematic uncertainties, expressed at the 98% confidence level. Above 60 eV for the K line an additional one sided uncertainty has been allowed for the possible presence of secondary electrons in the beam. Below 60 eV for the K line, the inner error bar represents the uncertainty excluding the uncertainty in the absolute optical calibration.

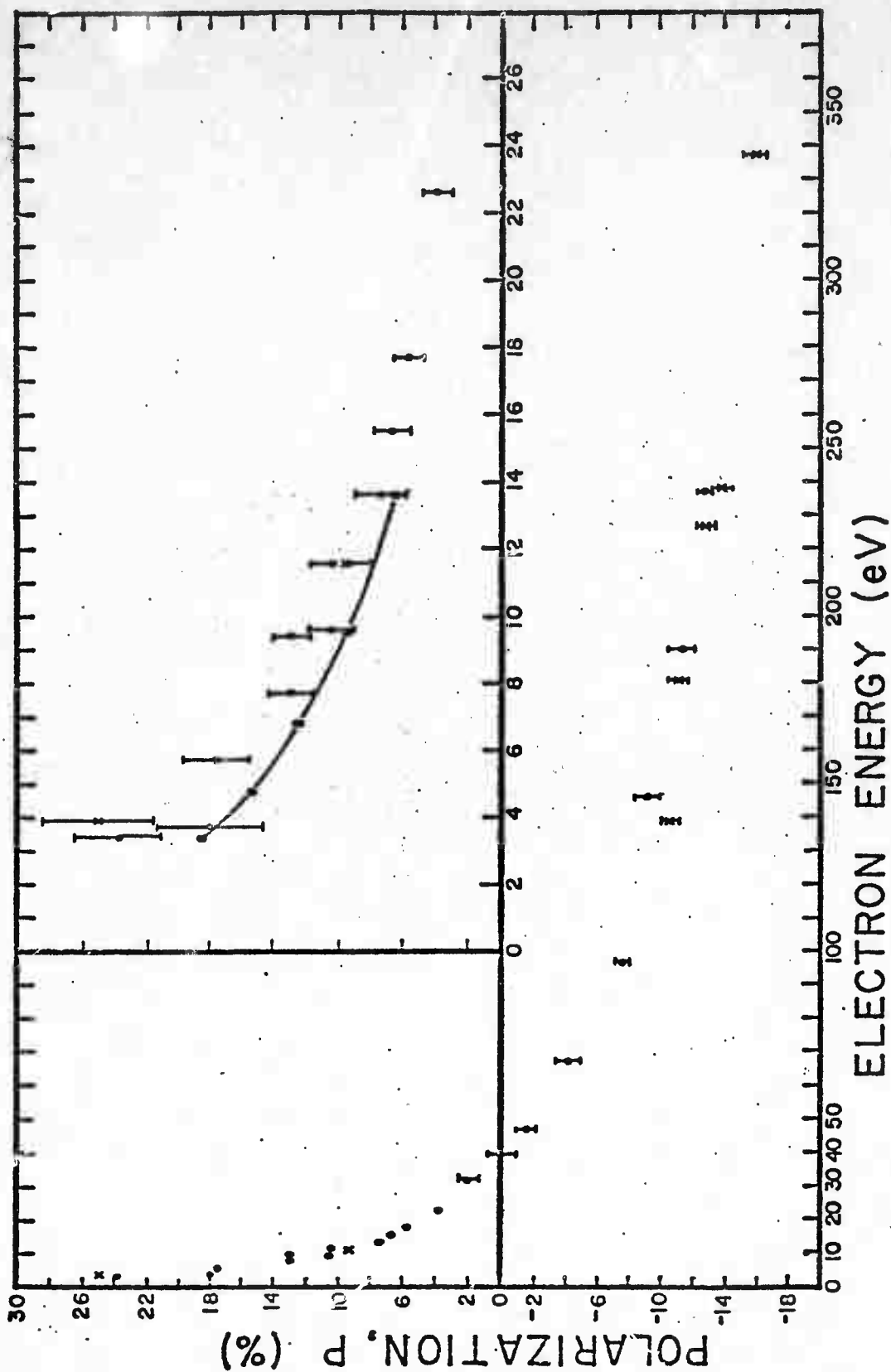


Fig. 6. Polarization of the K emission. The inset shows the low energy region on an expanded scale. Flags represent one S.D. of statistical fluctuations combined with systematic errors.
 x - Experimental data taken in 1972; 0 - Experimental data taken in 1970; -S- Theoretical polarization from Saraph (Ref. 3) based on the close coupling calculation of Burke and Moores (Ref. 1).

References

1. P. G. Burke and D. L. Moores, J. Phys. B (Proc. Phys. Soc.) 1, 575 (1968).
2. A. Burgess and V. J. Sheory, private communication, 1972.
3. H. E. Saraph, private communication, 1970.

Theoretical Atomic Physics (Dr. D. G. Hummer, Dr. J. I. Castor and Dr. D. W. Norcross).

The main emphasis in this period has been on the calculation of electron-excitation cross sections for CIII and NIV considering all transitions among the lowest 14 terms. Eleven configurations are included. Some progress has been made on the lithium-like ions CIV, NV and OVI using 9-term models. These cross sections are being calculated in the unitarized distorted-wave calculation. Much of the effort in this period has gone into improving the efficiency of the programs; as well, a considerable number of R-matrix elements have been calculated, although no cross sections have been finished to date.

We now have the capability to calculate resonance contributions to these cross sections which are ignored in the usual distorted wave procedure. As shown by Seaton,¹ multichannel quantum-defect theory allows one to use certain smoothly varying energy-dependent matrices, which can be computed in the distorted-wave approximation, to compute the resonance structure in electron-scattering cross sections. The code incorporating this analysis was written in London by a member of Professor Seaton's group and as a result of Hummer's recent visit to London and Seaton's visit to JILA, this facility is now operational here. It reproduces the results of coupled-equations calculations using about 1/100 of the computer time used by previously available techniques. The handling and final processing of the vast quantities of intermediate data involved now poses a serious problem and considerable effort is being spent on the design of an automatic data-handling procedure that is convenient yet reliable despite computer unreliability.

Reference

1. M. J. Seaton, J. Phys. B (Proc. Roy. Soc.) 2, 5 (1969).

Atomic Interaction Theory (Dr. S. Geltman and Dr. D. W. Norcross)

A general computer program has been prepared to calculate free-free absorption coefficients (inverse bremsstrahlung) and emissivities for neutral atoms. The continuum atomic wave functions are based on the Robinson-Geltman potential¹

$$U = U_{HS} + \frac{Z}{r} (1 - e^{-r/r_0}) - \alpha \frac{(1 - e^{-r/r_p})}{(r_p^2 + r^2)^2} \quad (1)$$

where U_{HS} is the Hartree-Fock-Slater potential as evaluated by the methods of Herman and Skillman,² the second term removes the Coulomb tail as seen by an electron within the neutral atom, and the third term is the polarization potential. The best available polarizabilities are taken from a recent complete tabulation,³ and the r_0 and r_p parameters are adjusted to give the best fit with elastic scattering data or electron affinities. All dipole matrix elements are evaluated numerically and enough partial waves are kept to insure convergence of results. Results are obtained for the atmospheric atoms N and O, as well as C and all the rare gases. The ranges of temperature and wavelength covered are $T = 500^\circ$ to $20000^\circ K$, $\lambda = .5$ to 20 microns. Comparison with the shock tube studies of Taylor and Caledonia⁴ shows good agreement for the case of Ne, while the shock tube results are about a factor of three higher than the present calculation for N, O, A, and Xe. We estimate the calculation to be good to about 30% on the basis of theoretical consistency and our fits to the scattering data. We plan to evaluate the free-free absorption coefficients of the metallic species Mg, Al, Si, Fe, and Ce.

Table I. Free-Free Atomic Absorption
Coefficients in Units of cm^5 .

Atom and Temperature	λ in Microns	Present Calculation	Taylor & Caledonia
Nitrogen 9175°K	2.0	8.86 (-39)	3.20 (-38)
	3.5	3.97 (-38)	1.30 (-37)
	5.0	1.08 (-37)	3.00 (-37)
Oxygen 9700°K	2.0	6.82 (-39)	2.90 (-38)
	3.5	3.12 (-38)	1.00 (-37)
	5.0	8.53 (-38)	2.60 (-37)
Neon 12600°K	2.0	5.40 (-39)	5.80 (-39)
	3.5	2.59 (-38)	2.70 (-38)
	5.0	7.21 (-38)	7.20 (-38)
Argon 9900°K	2.0	8.34 (-39)	3.80 (-38)
	3.5	3.81 (-38)	1.50 (-37)
	5.0	1.04 (-37)	3.60 (-37)
Xenon 8200°K	2.0	1.51 (-38)	3.00 (-38)
	3.5	6.50 (-38)	9.60 (-38)
	5.0	1.74 (-37)	2.00 (-37)

References

1. E. J. Robinson and S. Geltman, Phys. Rev. 153, 4 (1967).
2. F. Herman and S. Skillman, Atomic Structure Calculations (Prentice-Hall, 1963).
3. R. R. Trachant and R. L. Pack, Atomic Data 3, 195 (1971).
4. R. L. Taylor and G. Caledonia, J. Quant. Spectrosc. Radiative Transfer 9, 657, 681 (1969).

Electron scattering and photoionization. A paper on the close-coupling calculations of cross sections for low-energy (0-5 eV) scattering of electrons by sodium has been accepted for publication.¹ Additional experimental verification of these results has recently been obtained.²⁻⁴ These results are confined to elastic scattering from, and excitation of, the ground (3s) state. We are now proceeding to extract cross sections for elastic scattering from, excitation of, and transitions between the substates $3p(j=1/2)$ and $3p(j=3/2)$ of, the first excited state. Cross sections of the latter type are of particular importance in the developing field of infrared astronomy.

Reliable estimates of the photodetachment cross sections and electron affinities of the negative ions of the alkali metals are required for the interpretation of the properties of low-temperature plasmas. No reliable experimental data are available on the electron affinities of the alkali metals and none whatsoever on the photodetachment cross sections. Encouraged by the above results for sodium, photodetachment cross sections of the lithium and sodium negative ions have been computed for ejected electron energies from threshold to 5 eV ($\lambda \sim 20,000$ to 2000 \AA), using configuration-interaction (CI) wave functions⁵ for the initial states and solutions of the close-coupling equations for the final states. The results⁶ satisfy two "necessary" conditions quite well, and are significantly different from those of much less sophisticated calculations. A sharp resonant feature occurs in both cross sections at wavelengths corresponding to transitions to the first excited state of the neutral atom. This feature is so pronounced that it could be used for a precise determination of the electron affinities of lithium and sodium using present dye laser techniques. Equally reliable CI wave functions are available

for the negative ion of potassium,⁵ and these calculations will be extended to photodetachment of this species as soon as a suitable target model for the electron-potassium scattering calculation is obtained.

A study of photoabsorption by cesium has been completed.⁷ The results confirm the importance of the spin-orbit and core-polarization effects, and demonstrate that relativistic and non-adiabatic corrections omitted from previous work⁸ are not negligible. They also lend no support to a recent suggestion⁹ that there is a pole in the doublet line strength ratio for principal series transitions at principal quantum number $n \sim 10$ 15, and suggest that the accepted photoionization cross section¹⁰ is too large by about a factor of two. This work will be the basis of a close-coupling calculation of low-energy electron scattering by cesium, in an effort to resolve outstanding discrepancies between experimental and theoretical results.^{11,12} A similar study of photoabsorption by potassium will be undertaken for reasons discussed above.

References

1. D. L. Moores and D. W. Norcross, J. Phys. B: Atom. Molec. Phys. 5, in press.
2. K. Rubin, private communication.
3. A. Kasdan, T. M. Miller, and B. Bederson, private communication.
4. W. Gehenn and E. Reichert, Z. Phys., in press.
5. A. W. Weiss, Phys. Rev. 166, 70 (1968), and private communication.
6. D. W. Norcross and D. L. Moores, to be published in Atomic Physics III, Proceedings of the Third International Conference on Atomic Physics, Boulder (Plenum, New York, in press).
7. D. W. Norcross, Phys. Rev. A 5, 1621 (1972).

8. J. C. Weisheit, Phys. Rev. A 5, 1621 (1972).
9. G. Baum, M. S. Lubell, and W. Raith, Phys. Rev. A 5, 1073 (1972).
10. G. V. Marr and D. M. Creek, Proc. Roy. Soc. (London) A 304, 233 (1968).
11. P. J. Visconti, J. A. Slevin, and K. Rubin, Phys. Rev. A 3, 1310 (1971).
12. W. L. Nighan and A. J. Postma, to be published.

Ionizing Collisions (Dr. E. C. Beaty and Dr. J. Mauer)

Work was restarted on the project to study the energy and angular distributions of secondary electrons with the arrival of Dr. John Mauer. Some pieces of equipment failed during the shutdown, which combined with the new personnel has required redoing many of the equipment verification checks. This restarting procedure is nearly finished. Some extensions of the earlier data are planned. A new system for mounting the electron gun and a second detector have been designed and built. These new parts cannot be installed in the vacuum system until the present sequence of measurements is completed.

IV. GENERATION AND ABSORPTION OF RADIATION, ←

Program Leader - Dr. A. C. Gallagher

Alkali-Inert Gas Line Broadening and Intermolecular Potentials (Dr. A. C. Gallagher and Mr. D. L. Drummond)

The measurements of rubidium-inert gas spectra have been completed, and are being reduced to obtain the interaction potentials. In addition, undulations in these continuous spectra have been detected as shown by Fig. 7. These are attributed to transitions from bound vibrational states in the excited electronic state. Computations of bound-bound and bound-free Franck-Condon factors are now underway to utilize these data as a definite test of the adiabatic potentials inferred from the continuum data. Since these maxima in the continuum spectra identify vibrational states of the excited electronic state (the pressure dependence of the amplitudes of the maxima) can be used to test models for three-body molecular formation.

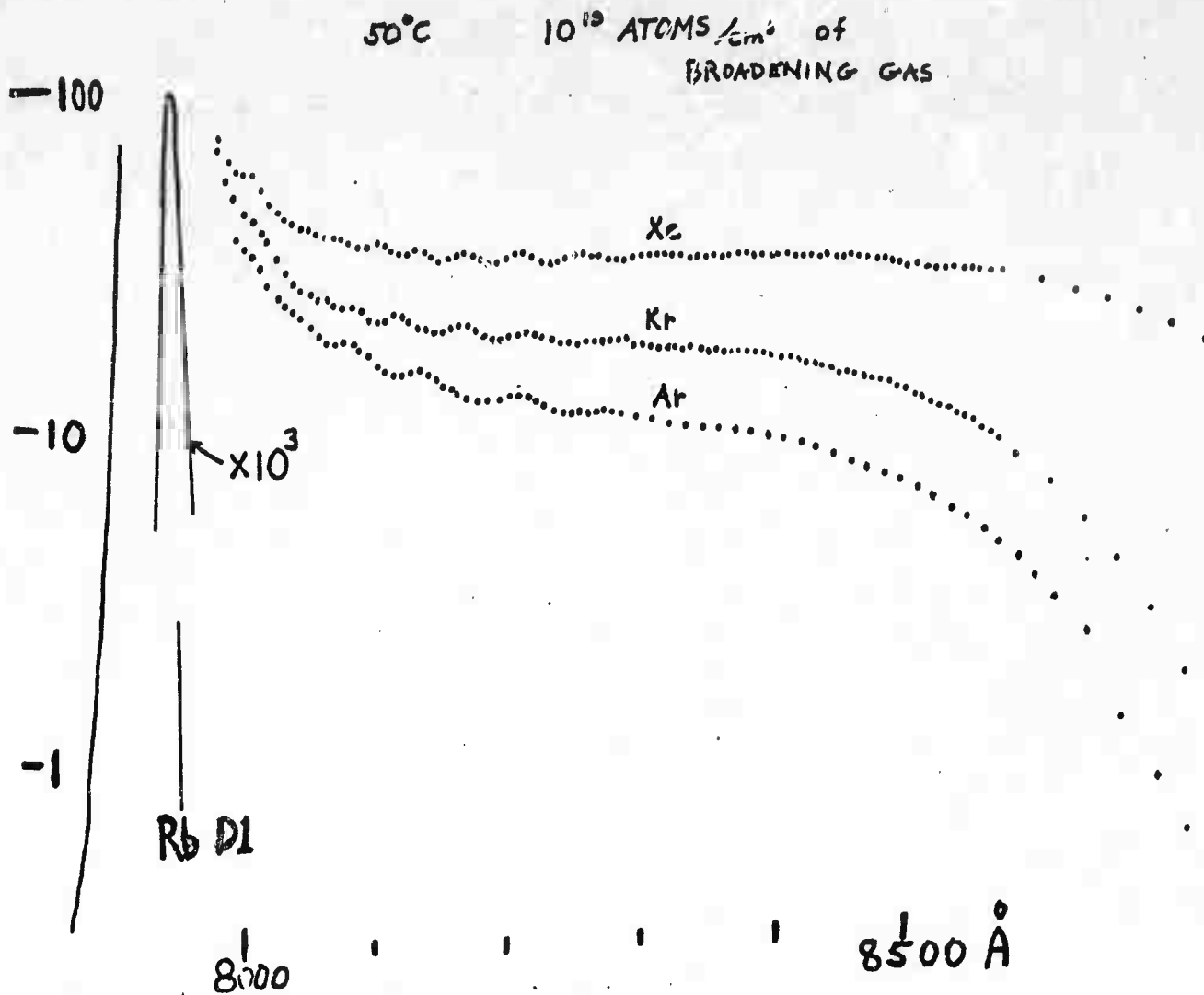


Figure 7. Emission spectrum of the rubidium resonance line perturbed by inert gases. The undulations are attributed to bound free transitions.

Plasma Spectroscopy (Dr. J. Cooper, Mr. J. Bauer, Mr. S. A. Freudenstein and Mr. J. Slater)

The theoretical work on the redistribution of radiation in the presence of collisions has been extended to take into account the effects of a magnetic field.¹ The results, which appear complicated, do however, lend themselves to simple physical interpretation in terms of magnetic field depolarization and multiple collision rates.

The tables on hydrogen line broadening have been accepted for publication,² and recent work on Stark broadening has concentrated on inclusion of ion dynamics. Preliminary results give excellent agreement with the HeI 4470 Å forbidden line. See Fig. 8.

Proton broadening of the wings of Lyman α has also been studied³ using accurate H_2^+ potentials. Of particular interest are various satellites which occur on the red wing at 1233.5, 1240.5 and 1409Å, as shown in Fig. 9.

Experimental work during this period has involved rebuilding equipment for obtaining high densities ($\approx 10^{15} \text{ cm}^{-3}$) of H^- for absorption experiments.

References

1. (I) A. Omont, J. Cooper and E. W. Smith, *Astrophys. J.* 175, 185 (1972).
(II) A. Omont, J. Cooper and E. W. Smith, in preparation.
2. C. R. Vidal, J. Cooper and E. W. Smith, *Astrophys. J. Suppl.* #215 (in press).
3. J. C. Stewart, J. M. Peek and J. Cooper, *Astrophys. J.* (in press).

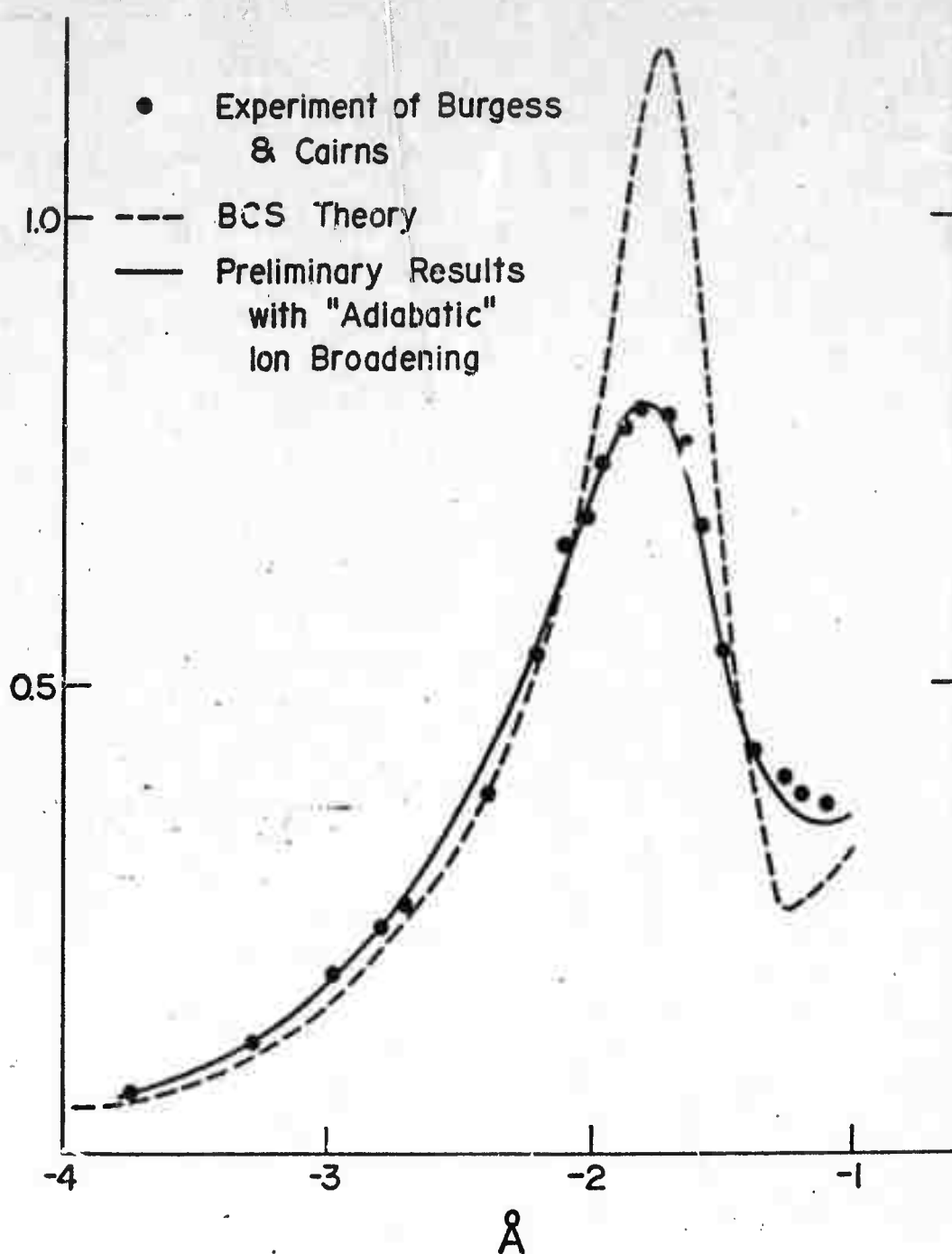


Fig. 8. Comparison of theory and experiment for HeI 4470Å $2^3P - 4^3F$.

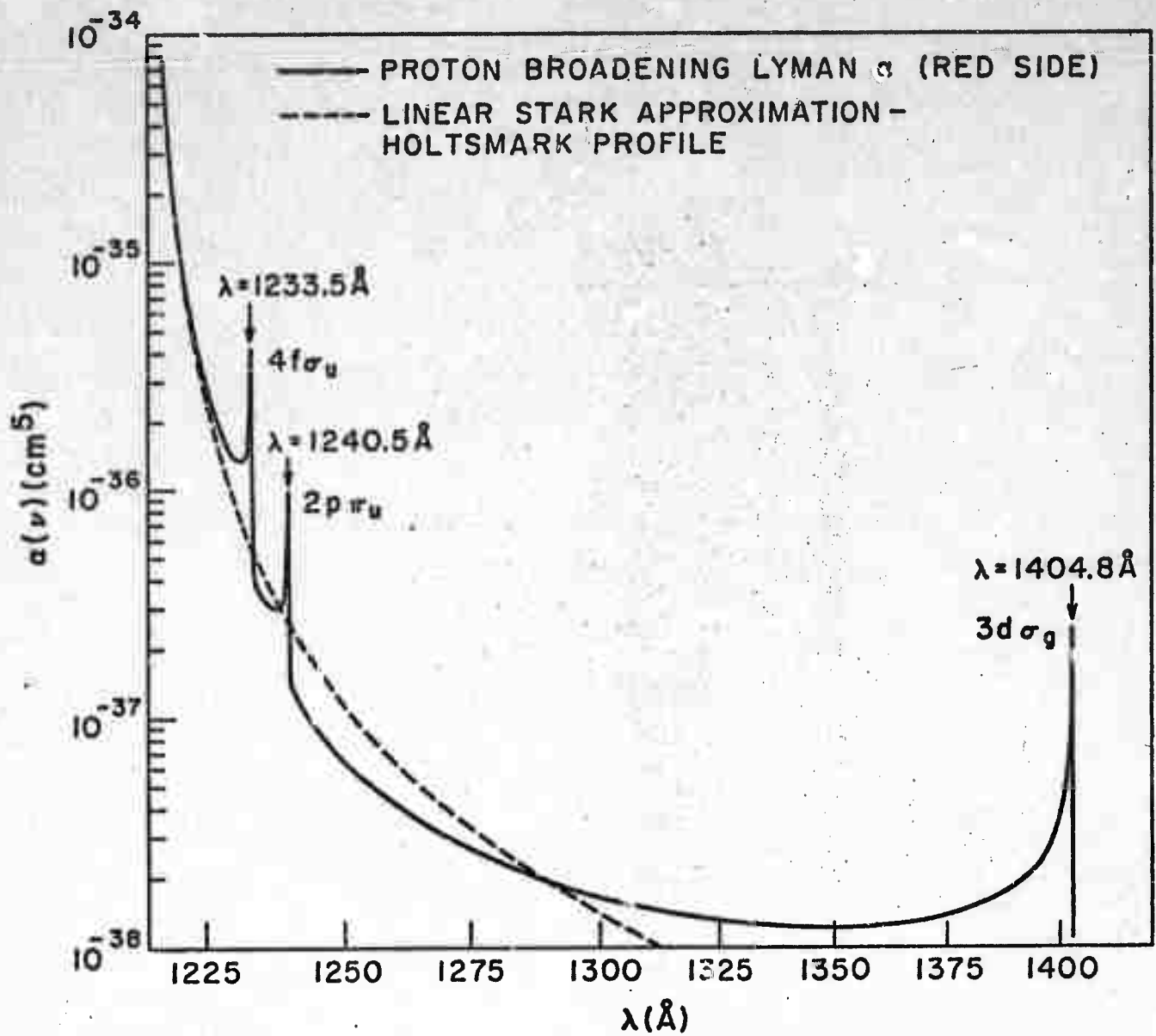


Fig 9. Absorption coefficient α for red wing of Lyman α . The Holtzmark profile is shown.

Prediction of Laser Gain (Dr. A. V. Phelps)

The theory and understanding developed during the study of alkali-inert gas broadening and intermolecular potentials, as discussed above, has been applied to the prediction of the gain of proposed laser systems utilizing molecules with dissociating ground states, e.g., Xe_2 or LiXe . Thus, we have utilized theoretically or experimentally determined intermolecular potential energy curves for the ground state and first excited state of molecules to calculate the magnitude and spectral variation of absorption and stimulated emission coefficients. These calculations show that the densities of excited molecules required for lasers of reasonable length are high, e.g., of the order of 10^{15} molecules/cm³, but are apparently attainable with sufficiently intense excitation. Figure 10 shows results obtained for the LiXe system. A detailed discussion of these results has been prepared and will be sent to those on the ARPA distribution list as JILA Report 110.

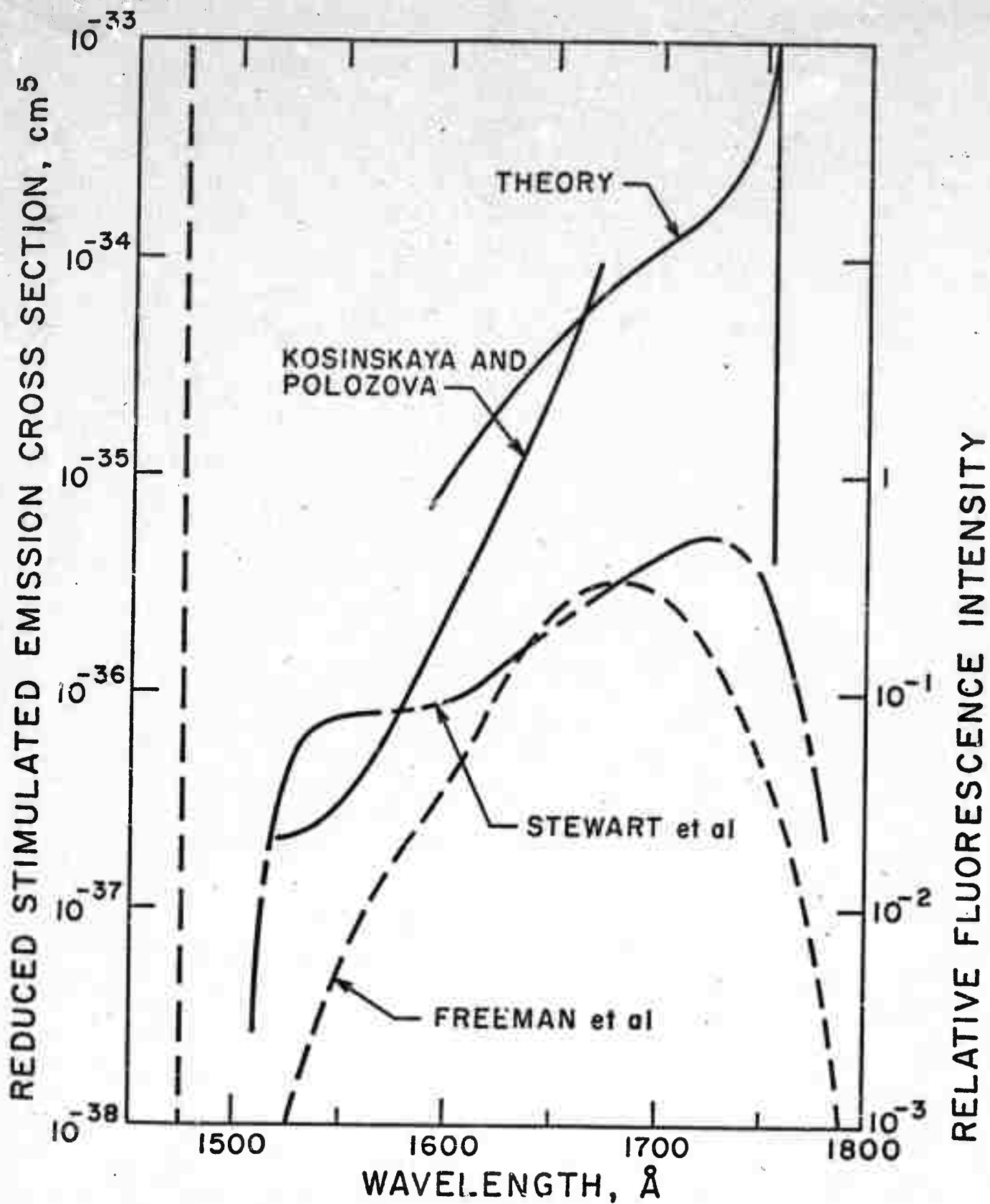


Fig. 10. Stimulated emission and fluorescence in xenon.

Manuscripts Involving ARPA Funds

Listed below are papers submitted for publication during the period covered by this report. Co-authors not connected with JILA are shown in parentheses.

- R. A. Bennett and J. L. Hall, "Electron affinity of SO by laser photo-detachment," Bull. Am. Phys. Soc. 17, 574 (1972) [Abstract].
- W. R. Chappell and (R. H. Williams), "Kinetic theory of partially ionized gases," Bull. Am. Phys. Soc. 17, 78 (1972) [Abstract].
- J. L. Hall and R. L. Barger, "Line shape effects in saturated absorption," Bull. Am. Phys. Soc. 17, 67 (1972) [Abstract].
- R. E. M. Hedges, D. L. Drummond and A. Gallagher, "Extreme wing line broadening and Cs-inert gas potentials," submitted to Phys. Rev. A.
- H. Hotop, T. A. Patterson, and W. C. Lineberger, "High resolution photo-detachment studies of Se⁻," Bull. Am. Phys. Soc. 17, 150 (1972) [Abstract].
- J. A. Jenkins and A. V. Phelps, "Measurement of the self broadened wings of the potassium D₁ and D₂ lines," to appear in Bull. Am. Phys. Soc. [Abstract].
- L. J. Kieffer (Editor), "Proceedings of the Workshop on Dissociative Excitation of Simple Molecules," JILA Information Center Report No. 12, June 1, 1972.
- J. A. Magyar and J. L. Hall, "Saturated absorption optical heterodyne spectroscopy of simple methyl compounds," Bull. Am. Phys. Soc. 17, 67 (1972) [Abstract].
- B. W. Woodward, W. C. Lineberger and L. M. Branscomb, "Ionization of cesium atoms in collisions with atomic oxygen," submitted to Phys. Rev. A.